

3-Methoxybutyl acetate  
4435-53-4 | DTXSID2052106

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 23.4 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.94e-01

Confidence level: 5.78e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Methoxy-2-propyl acetate</div> <div>Measured: 2.29</div> <div>Predicted: 7.33</div>	<div>Image not found</div> <div>N-Methyl-N'-phenylurea</div> <div>Measured: 19.5</div> <div>Predicted: 29.8</div>	<div>Image not found</div> <div>Urea, (3-methylphenyl)-</div> <div>Measured: 36.3</div> <div>Predicted: 37.2</div>
<div>Image not found</div> <div>Ethyl valerate</div> <div>Measured: 93.3</div> <div>Predicted: 68.6</div>	<div>Image not found</div> <div>2-Butoxyethanol</div> <div>Measured: 67.6</div> <div>Predicted: 45.0</div>	